Metal–insulator transition in the antiferromagnetic state of the Hubbard model: analytical theory

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Metal–insulator transition in the antiferromagnetic state of the Hubbard model: analytical theory

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Abstract. In the framework of numerical calculations and analytical expansion in the transfer integral between the next-nearest neighbors t' and the direct antiferromagnetic (AFM) gap Δ, the metal–insulator transition criterion is obtained, the Hartree-Fock and slave boson approaches being used. In the case of a square lattice, there is an interval of t' values, for which the metal-insulator transition is a first-order transition, which is due to the Van Hove singularity near the center of the band. For simple and body-centered cubic lattices, the transition from the insulator AFM state occurs to the phase of an AFM metal and is a second-order phase transition; it is followed by a transition to a paramagnetic metal. These results are modified when taking into account the intersite Heisenberg interaction which can induce first-order transitions.

1. Introduction

The nature of the metal—insulator transition in strongly correlated systems is still not understood in detail. The competition between the insulator antiferromagnetic (AFM) state and the paramagnetic one gives the phase boundary of the metal—insulator transition of the first order [1]. However, taking into account the transfer between the second neighbors can lead to the appearance of the AFM metallic phase which may be more energetically favorable than the paramagnetic metal. Thus the first-order transitions do not occur for the three-dimensional simple and body-centered cubic lattices in the Hubbard model with on-site repulsion [2]. At the same, the situation can change when taking into account intersite interactions in the extended Hubbard model (see, e.g., Ref. [3]).

In the present work we treat these issues by using the slave boson approach [4] in a generalized $t - t'$ Hubbard model including intersite exchange interactions. We take into account Van Hove singularities of electron spectrum and obtain the ground-state metal–insulator transition criterion within the framework of an analytical expansion in the next-nearest neighbor transfer integral t' and direct AFM gap Δ.

2. Model and theory

We use the Hubbard Hamiltonian with inclusion of direct exchange interaction:

$$\mathcal{H}_{\mathrm{H}} = \sum_{ij\sigma} t_{ij} c^{\dagger}_{i\sigma} c_{j\sigma} + U \sum_{i} n_{i\uparrow} n_{i\downarrow} + \frac{1}{2} \sum_{ij} J_{ij} \mathbf{S}_i \mathbf{S}_j, \tag{1}$$

with the electron hopping $t_{ij} = -t$ for the nearest neighbors and t' for the next-nearest neighbors (we assume $t > 0$), $c^\dagger_{i\sigma}, c_{i\sigma}$ the electron creation and annihilation operators, $\mathbf{S}_i = (1/2)\sum_{\sigma\sigma'} c^\dagger_{i\sigma}\vec{\sigma}_{\sigma\sigma'}c_{i\sigma'}$. We apply the slave boson representation proposed by Kotliar and Ruckenstein [4] and generalized [5] on the case of spiral magnetic ordering

$$\langle \mathbf{S}_i \rangle = (m/2)(\hat{\mathbf{z}}\cos\mathbf{Q}\mathbf{R}_i + \hat{\mathbf{y}}\sin\mathbf{Q}\mathbf{R}_i) \tag{2}$$

through local rotation around x axis in spin space: $c_{i\sigma} \to \sum_{\sigma'}\exp(\mathrm{i}\sigma_x\mathbf{Q}\mathbf{R}_i/2)_{\sigma\sigma'}c_{i\sigma'}$ to match the magnetization direction with z axis. A simple way of taking into account the correlation effects is an extension of the configuration space to a bosonic sector by introducing the *slave-boson* annihilation (creation) operators $e_i(e^\dagger_i)$, $p_{i\sigma}(p^\dagger_{i\sigma}), d_i(d^\dagger_i)$ for empty, singly and doubly occupied states, respectively, so that

$$c^\dagger_{i\sigma} \to f^\dagger_{i\sigma}z^\dagger_{i\sigma} \tag{3}$$

where $f_{i\sigma}, f^\dagger_{i\sigma}$ are the Fermi operators, and

$$z^\dagger_{i\sigma} = (1 - e^\dagger_i e_i - p^\dagger_{i\bar{\sigma}}p_{i\bar{\sigma}})^{-1/2}(p^\dagger_{i\sigma}e_i + d^\dagger_i p_{i\bar{\sigma}})(1 - d^\dagger_i d_i - p^\dagger_{i\sigma}p_{i\sigma})^{-1/2} \tag{4}$$

is a site transition operator acting in bosonic subspace, $\bar{\sigma} = -\sigma$. The coherence of bosonic and fermionic description is achieved by constraints

$$e^\dagger_i e_i + \sum_\sigma p^\dagger_{i\sigma}p_{i\sigma} + d^\dagger_i d_i = 1, \tag{5}$$

$$d^\dagger_i d_i + p^\dagger_{i\sigma}p_{i\sigma} = f^\dagger_{i\sigma}f_{i\sigma}. \tag{6}$$

Under these constraints we express the interaction terms in (1) in the boson language: $n_{i\uparrow}n_{i\downarrow} \to d^\dagger_i d_i$, $\mathbf{S}_i \to (1/2)\sum_{\sigma\sigma'} p^\dagger_{i\sigma}\vec{\sigma}_{\sigma\sigma'}p_{i\sigma'}$.

In the saddle point approximation we pass to c-number bosonic amplitudes e, p_σ, d ($e_i, e^\dagger_i \to e$ etc.) which are determined from the equations

$$n = 2d^2 + p^2_\uparrow + p^2_\downarrow, \tag{7}$$

$$m = p^2_\uparrow - p^2_\downarrow, \tag{8}$$

$$1 = e^2 + p^2_\uparrow + p^2_\downarrow + d^2, \tag{9}$$

$$U = \frac{-\zeta}{edp_\uparrow p_\downarrow}\sum_\sigma \frac{(ep_\uparrow + p_\downarrow d)(ep_\downarrow + p_\uparrow d)}{(e^2 + p^2_{\bar{\sigma}})(p^2_\sigma + d^2)}\Phi_\sigma, \tag{10}$$

where n is electron concentration,

$$\zeta = p_\uparrow p_\downarrow - ed \tag{11}$$

is correlation strength parameter,

$$z^2_\sigma = 1 - \frac{\zeta^2}{(e^2 + p^2_{\bar{\sigma}})(p^2_\sigma + d^2)}, \tag{12}$$

is a local band narrowing factor. Then Φ_σ, n and m are determined by lattice sums

$$\Phi_\sigma = \frac{1}{2N}\sum_{\mathbf{k}s} e_+(\mathbf{k})f_{\mathbf{k}s} + \frac{1}{2N}\sum_{\mathbf{k}s}\frac{(-1)^s\left(-\sigma e_+(\mathbf{k})\bar{\Delta}_{\mathbf{k}} + e^2_-(\mathbf{k})z^2_{\bar{\sigma}}\right)f_{\mathbf{k}s}}{\sqrt{\bar{\Delta}^2_{\mathbf{k}} + z^2_\uparrow z^2_\downarrow e^2_-(\mathbf{k})}}, \tag{13}$$

$$n = \frac{1}{N}\sum_{\mathbf{k}s} f_{\mathbf{k}s}, \tag{14}$$

$$m = \frac{1}{N}\sum_{\mathbf{k}s} \frac{(-1)^{s+1}\bar{\Delta}_{\mathbf{k}} f_{\mathbf{k}s}}{\sqrt{\bar{\Delta}^2_{\mathbf{k}} + z^2_\uparrow z^2_\downarrow e^2_-(\mathbf{k})}}, \tag{15}$$

where $\bar{\Delta}_{\mathbf{k}} = \Delta - (z^2_\uparrow - z^2_\downarrow)e_+(\mathbf{k})/2$, $f_{\mathbf{k}s} = f(E_s(\mathbf{k}))$, $f(E)$ being the Fermi function,

$$E_s(\mathbf{k}) = \frac{1}{2}(z^2_\uparrow + z^2_\downarrow)e_+(\mathbf{k}) + \lambda + (-1)^s\sqrt{\bar{\Delta}^2_{\mathbf{k}} + z^2_\uparrow z^2_\downarrow e^2_-(\mathbf{k})},\ s = 1, 2 \tag{16}$$

are antiferromagnetic subbands of slave fermions. Here $e_\pm(\mathbf{k}) = (t_{\mathbf{k}} \pm t_{\mathbf{k}+\mathbf{Q}})/2$, so that $e_+(\mathbf{k}) \propto t', e_-(\mathbf{k}) \propto t$.

The Fermi level shift λ and AFM gap Δ produced by interaction obey the equations

$$\lambda = \frac{U}{2} + \frac{\zeta}{2ed}\sum_\sigma \frac{ep_\sigma + p_{\bar{\sigma}}d}{(e^2 + p^2_{\bar{\sigma}})(p^2_\sigma + d^2)}\left(\frac{ep_\sigma}{p^2_\sigma + d^2} - \frac{dp_{\bar{\sigma}}}{e^2 + p^2_{\bar{\sigma}}}\right)\Phi_\sigma, \tag{17}$$

$$\Delta + \frac{J_{\mathbf{Q}}m}{4} = -\frac{\zeta}{2p_\uparrow p_\downarrow}\sum_\sigma \frac{\sigma(ep_\sigma + p_{\bar{\sigma}}d)}{(e^2 + p^2_{\bar{\sigma}})(p^2_\sigma + d^2)}\left(\frac{ep_\sigma}{e^2 + p^2_{\bar{\sigma}}} - \frac{p_{\bar{\sigma}}d}{p^2_\sigma + d^2}\right)\Phi_\sigma. \tag{18}$$

Within the Hartree-Fock approximation (HFA) these quantities are determined in a much simpler way: $\zeta = 0$, $\lambda = Un/2$ and $\Delta = U_{\text{eff}}(\mathbf{Q})m/2$, where

$$U_{\text{eff}}(\mathbf{Q}) = U - J_{\mathbf{Q}}/2, \tag{19}$$

$$J_{\mathbf{q}} = (1/N)\sum_{ij} J_{ij}\exp(\mathrm{i}\mathbf{q}\mathbf{R}_i). \tag{20}$$

For half-filled case we have $z^2_{\text{AFM}} = z^2_\sigma = 1 - 4\zeta^2_{\text{AFM}}/(1 - m^2), e = d$ and, provided that the AFM insulator state is assumed to occur, the equations are simplified:

$$m = \Delta_*\Phi_1(\Delta_*), \tag{21}$$

$$\Delta_* - \frac{2\bar{J}m}{1 - 4\zeta^2_{\text{AFM}}/(1 - m^2)} = \frac{Um}{2}\frac{1 + \zeta_{\text{AFM}}}{(1 + 2\zeta_{\text{AFM}})^2}, \tag{22}$$

$$\frac{16\zeta_{\text{AFM}}(1 + 2\zeta_{\text{AFM}})^2}{(1 - m^2)((1 + 2\zeta_{\text{AFM}})^2 - m^2)}\Phi_2(\Delta_*) = U, \tag{23}$$

where $\Delta_* = \Delta/z^2_{\text{AFM}}$. For simplicity we take exchange integral J_{ij} in the nearest-neighbor approximation, $\bar{J} = ZJ/8$, Z being nearest-neighbor number. The lattice sums

$$\Phi_1(\Delta) = \frac{1}{N}\sum_{\mathbf{k}} \frac{1}{\sqrt{\Delta^2 + e^2_-(\mathbf{k})}}, \tag{24}$$

$$\Phi_2(\Delta) = \frac{1}{N}\sum_{\mathbf{k}} \frac{e^2_-(\mathbf{k})}{\sqrt{\Delta^2 + e^2_-(\mathbf{k})}} \tag{25}$$

are determined by the $e_-(\mathbf{k})$ component of the spectrum only. The corresponding free energy reads

$$F_{\text{AFM}} = -\bar{J}m^2 + z^2_{\text{AFM}}\left(\frac{U}{4}\frac{1 - m^2}{1 + 2\zeta} - \Phi_2(\Delta_*)\right). \tag{26}$$

The expression (26) contains contributions from both the Coulomb interaction and the intersite exchange interaction. In this case, unlike HFA, these contributions work in different ways: the Coulomb contribution to F_{AFM} contains an additional "correlation" factor, depending on ζ.

The insulator AFM phase competes with the paramagnetic and antiferromagnetic metal phases. Since at half-filling the correlation narrowing of the spectrum occurs uniformly by the factor z^2_{AFM}, we have for the gap at the boundary of the transition into AFM metal

$$\Delta = z^2_{\mathrm{AFM}}\Delta_{\mathrm{MIT}}(\tau)$$

where $\tau = t'/t$ and for the square lattice

$$\Delta^{\mathrm{sq}}_{\mathrm{MIT}}(\tau) = t\begin{cases}2\tau, & \tau < 1/\sqrt{2},\\ 4\tau - \tau^{-1}, & \tau > 1/\sqrt{2}.\end{cases}; \tag{27}$$

for the sc lattice

$$\Delta^{\mathrm{sc}}_{\mathrm{MIT}}(\tau) = t\begin{cases}2\tau, & \tau < \sqrt{3}/4,\\ 8\tau - 9\tau^{-1}/8, & \tau > \sqrt{3}/4.\end{cases}; \tag{28}$$

and for bcc lattice

$$\Delta^{\mathrm{bcc}}_{\mathrm{MIT}}(\tau) = t\begin{cases}4\tau, & \tau < 2/\sqrt{3},\\ 6\tau - 8\tau^{-1}/3, & \tau > 2/\sqrt{3}.\end{cases}. \tag{29}$$

Unlike the free energy of the AFM insulator phase, the free energy of the paramagnetic (PM) phase essentially depends on τ:

$$F_{\mathrm{PM}} = \frac{U}{4}(1 - \zeta_{\mathrm{PM}}) + \mathcal{E}(\tau), \tag{30}$$

where $\zeta_{\mathrm{PM}} = -U/(16\mathcal{E}(\tau))$ and

$$\mathcal{E}(\tau) = (2/N)\sum_{\mathbf{k}} t_{\mathbf{k}}(\tau) f(t_{\mathbf{k}}(\tau)), \tag{31}$$

where the paramagnetic phase Fermi level is adjusted to obey $n = 1$.

To determine the type of MIT, it is convenient to consider the energy difference between the AFM insulator and the PM metal ΔF_{MIT} at the boundary AFM metal—AFM insulator $\Delta_* = \Delta_{\mathrm{MIT}}(\tau)$ [see (27), (28), (29)]. We have

$$\Delta F_{\mathrm{MIT}}(\tau) = \frac{U(\zeta_{\mathrm{PM}} - \zeta_{\mathrm{AFM}})}{4} + \frac{Um^2\zeta_{\mathrm{AFM}}(1 + 4\zeta_{\mathrm{AFM}})}{4(1 + 2\zeta_{\mathrm{AFM}})^2} + \Delta F^{\mathrm{HFA}}_{\mathrm{MIT}}(\tau), \tag{32}$$

where the free energy difference at MIT boundary within HFA (within this approximation $\Delta_* = \Delta$, $\zeta = 0$ for both phases),

$$\Delta F^{\mathrm{HFA}}_{\mathrm{MIT}}(\tau) = -\bar{J}m^2 + \delta\mathcal{F} - \delta\mathcal{E}(\tau), \tag{33}$$

with $\delta\mathcal{F} = -Um^2/4 - \delta\Phi_2(\Delta_*)$ being the AFM energy change within HFA (without exchange contribution), $\delta\mathcal{E}(\tau) = \mathcal{E}(\tau) + \Phi_2(0), \delta\Phi_2(\tau) = \Phi_2(\tau) - \Phi_2(0)$. If $\Delta F_{\mathrm{MIT}} > 0$, the direct transition from AFM insulator into PM metal phase occurs, and this is the first-order phase transition. Otherwise, this transition occurs through the a pair of second order transitions including the metallic AFM phase.

After expanding in Δ_* and ζ, Eq. (32) takes the form

$$\Delta F_{\rm MIT} = \frac{U\zeta_0(3-4\zeta_0)m^2}{4} + \left(1-48\zeta_0^2\right)\Delta F_{\rm MIT}^{\rm HFA}, \tag{34}$$

with

$$\zeta_0 = \frac{\Phi_1^{-1}(\Delta_*) - \bar{J}}{U_{\rm BR}}, \tag{35}$$

$U_{\rm BR} \equiv U_{\rm BR}(0) = 8\Phi_2(0)$, $U_{\rm BR}(\tau) = -8\mathcal{E}(\tau)$ being the critical MIT value in the paramagnetic state [7].

The critical value $U = U_{\rm MIT}$ at the MIT boundary reads

$$U_{\rm MIT} = 2(\Phi_1^{-1}(\Delta_*) - \bar{J})(1+3\zeta_0), \tag{36}$$

ζ_0 term being a positive correlation correction. It follows from Eq. (34) that the correlation correction, proportional to ζ_0, leads to a larger increase in the energy of the AFM insulator phase than of the PM phase. This means that the correlation contributions expand the first-order transition region, or even can turn the second-order transition into a first-order transition.

To leading order in ζ and Δ we derive

$$\Delta F_{\rm MIT} = \delta\mathcal{F} - \delta\mathcal{E}(\tau) - \bar{J}\Phi_1^2(\Delta_*))\Delta_*^2 + \frac{3\Delta_*^2}{2U_{\rm BR}}(1-\bar{J}\Phi_1(\Delta_*))^2, \tag{37}$$

where the AFM energy change is presented in the form $\delta\mathcal{F} = \Delta_*^3 G'(\Delta_*)/2$,

$$G(\Delta) = \frac{1}{N}\sum_{\mathbf{k}} \frac{1}{\sqrt{\Delta^2 + e_-^2(\mathbf{k})} + |e_-(\mathbf{k})|}. \tag{38}$$

The third term in (37) is the leading contribution to the change in energy from the exchange interaction, the fourth term is the correlation correction. Taking into account the direct exchange interaction in the framework of the Hartree-Fock approximation will lead to the replacement of U by $U_{\rm eff}(\mathbf{Q})$ only, which cannot change the type of transition. Therefore we should work with account of correlation effects which change the situation.

The role of the exchange correction depends on the sign of J: antiferromagnetic exchange stabilizes the AFM state expanding the region of the second order transition, and the ferromagnetic exchange destabilizes it and leads to first-order transition.

3. Results

At half filling, the dependence of the energy of the paramagnetic and AFM insulator states on the model parameters is determined mainly by the behavior of the density of electronic states in the vicinity of the center of the band. Here we can distinguish two cases: (a) a nonsingular density of states (e.g., simple cubic lattice), when this energy has a quadratic dependence on the parameters t' or the AFM gap Δ, and (b) the singular density of states (e.g., square and bcc lattice), when this quadratic dependence acquires additional logarithmic factors and, thus, is essentially non-analytic.

The τ dependence of $U_{\rm MIT}$ for different lattices in the absence of correlations is shown in Fig. 1. It is clear that different behaviour of density of state in the vicinity of the band center results in very different dependence of $U_{\rm MIT}(\tau)$,

$$1/U_{\rm MIT} = \begin{cases} \rho(0)\ln(D/D'), & \rho(E)\sim\rho(0) \\ (a/2)\ln^2(D/D'), & \rho(E)\sim a\ln(D/|E|), \\ (a'/3)\ln^3(D/D'), & \rho(E)\sim a'\ln^2(D/|E|) \end{cases}, \tag{39}$$

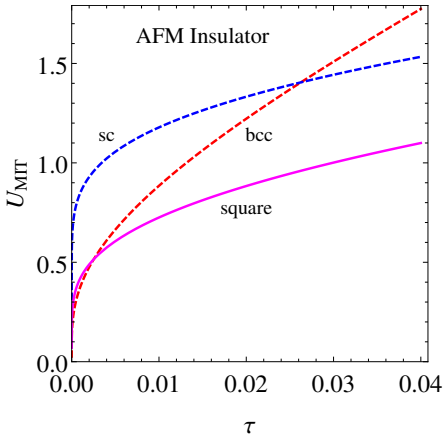

Figure 1. The transition boundary of the AFM metal — AFM insulator for various lattices according to (36) for $U_{\rm MIT}(\tau)$ in HFA ($J = \zeta_0 = 0$).

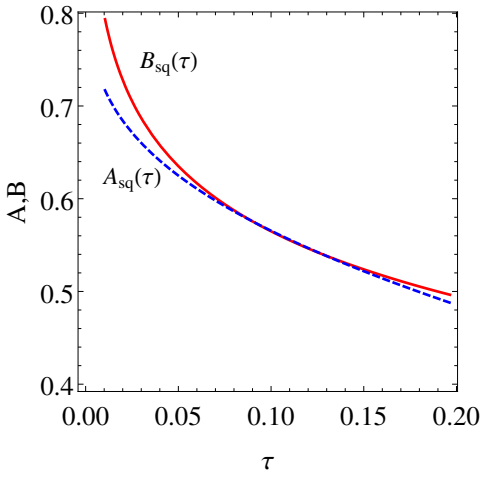

Figure 2. The dependence of expansion coefficients $A_{\rm sq}(\tau), B_{\rm sq}(\tau)$ on the MIT boundary in the AFM phase on the square lattice.

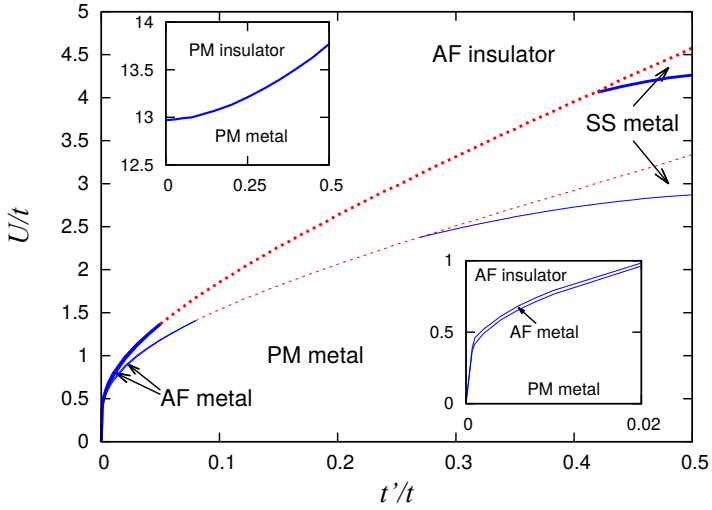

Figure 3. The magnetic phase diagram of the ground state of the Hubbard model at half filling in the τ plane is U/t for a square lattice [2]. Thick (thin) lines represent the result of SBA (HFA). Solid (dashed) lines are the second (first) order transition lines. The bottom box shows the phase diagram obtained in the SBA, in particular, for small t'. The upper inset is the result of the Brinkman-Rice result $U_{\rm MIT} = U_{\rm BR}(\tau)$ [7] (transition in the PM phase).

where $a, a,'$ are positive constants, D' is an energy scale of next-nearest neighbour hopping.

The general expansion of $G(\Delta)$

$$G(\Delta) = D^{-1}\left(a_0 + a_1 \ln\frac{2D}{\Delta} + a_2 \ln^2\frac{2D}{\Delta}\right), \tag{40}$$

allows to obtain expansions for quantities entering Eqs. (21),(22), (23)

$$\Phi_1(\Delta) = 2G(\Delta) + \Delta G'(\Delta), \tag{41}$$
$$\Phi_2(\Delta) = \Phi_2(0) - \Delta^2(G(\Delta) + \Delta G'(\Delta)). \tag{42}$$

For the square lattice ($D_{\rm sq} = 4t, U^{\rm sq}_{\rm BR} = 13.0t$) the density of states in the vicinity of the center of the band contains a logarithmic contribution, so that

$$a_0^{\rm sq} = \left(\frac{3+\pi^2}{6} + 2\ln 2\right)/\pi^2 + \delta g_{\rm sq}\,, a_1^{\rm sq} = \frac{1+4\ln 2}{\pi^2}\,, a_2^{\rm sq} = \pi^{-2}$$

where $\delta g_{\rm sq} = 0.02805$.

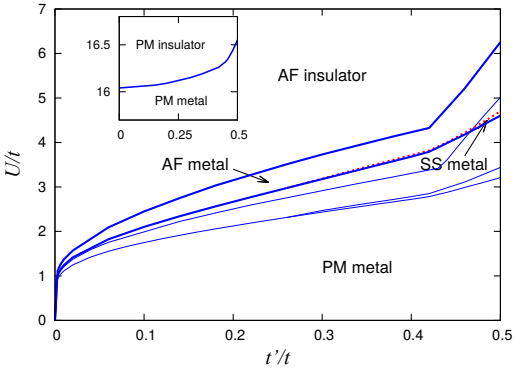

Figure 4. The same as for Fig. 3 for sc lattice phase labels are addressed to SBA only [2].

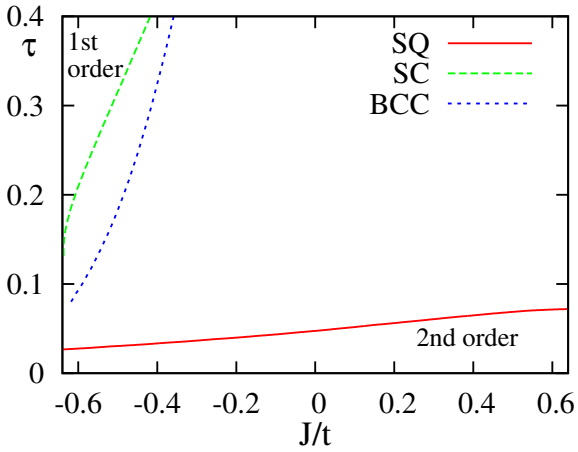

Figure 5. The phase diagram demonstrating the MIT type in the $J-\tau$ variables for square (SQ), simple cubic (SC) and body centered cubic (BCC) lattices, J is the exchange integral between the nearest neighbors. To the left of the curves, a first order transition takes place, to the right – the second order transition.

The Van Hove singularity leads to an additional singular (logarithmic) contribution to the energy of the AFM and PM states and a contribution of the order of $\ln^2(t/\Delta)$ to the inverse critical value U. The dependence of $U^{\rm sq}_{\rm MIT}$ and $\delta\mathcal{F}_{\rm sq}$ on τ at the MIT boundary and the effect of exchange and correlation corrections can be obtained from the formula (35), (36), and (40) using the asymptotic result at small τ up to leading terms

$$\Phi_1^{\rm sq}(\Delta_{\rm MIT}(\tau)) = \frac{1}{2\pi^2 t}\ln^2\frac{16}{\tau}, \quad (43)$$

$$\delta\mathcal{F}_{\rm sq}(\Delta_{\rm MIT}(\tau)) = -B_{\rm sq}(\tau)\tau^2 t, \quad (44)$$

where $B_{\rm sq}(\tau) = \left(1+2\ln\frac{16}{\tau}\right)/(2\pi^2)$.

The dependence of the energy of the PM phase on τ contains non-analytic contributions arising from the singularity inside the band, which is present for any τ,

$$\delta\mathcal{E}_{\rm sq}(\tau) = -A_{\rm sq}(\omega_{\rm F})\tau^2 t, \quad (45)$$

where

$$A_{\rm sq}(\omega) = \bar{A}_{\rm sq} - \frac{32/\pi^2}{1+\ln(16/\omega)} + \frac{16/\pi^2}{(1+\ln(16/\omega))^2}, \quad (46)$$

$\bar{A}_{\rm sq} = 1.08, \omega_{\rm F} = E_{\rm F}/t + 4\tau$ is the Fermi energy measured from the Van Hove singularity position.

From Fig. 2 one can see that $B_{\rm sq}(\tau) > A_{\rm sq}(\tau)$ with the exception of a small interval. For very small τ, the insulator phase appears to be more favourable than the paramagnetic one due to the logarithmic contribution to energy. However, as Δ increases, the phase energies intersect at two points $\tau_{1,2}$. The intersection at $\tau = \tau_2$ is an expansion artifact and is absent when equations are numerically solved: with $\tau > \tau_1$, the MIT becomes a first-order transition (Fig. 3). The closeness of the coefficients $A_{\rm sq}(\tau)$ and $B_{\rm sq}(\tau)$ is an indication of the existence of only a narrow AFM metal region between the AFM insulator and PM of the metal on the phase diagram.

Fig. 3 shows the results of numerical solution of both HFA and slave boson approach (SBA) equations for the square lattice with $J = 0$ with account of non-collinear AFM (spiral) order [2]. One can see that large enough τ values favor first-order MIT transition, and the correlation effects considerably enlarge the first-order transition region.

The nonlinear relationship between Δ and τ at the boundary of the AFM insulator – PM metal transition owing to the singularity leads to a change in the type of transition from the second to the first order at $\tau \simeq 0.05$ (within HFA, 0.08); numerically, this result was obtained earlier [8, 2].

For the simple cubic lattice ($D_{\rm sc} = 6t, U^{\rm sc}_{\rm BR} = 16.0t$)

$$a^{\rm sc}_0 = D_{\rm sc}\rho_{\rm sc}(0)/2 + \delta g_{\rm sc}, \quad (47)$$
$$a^{\rm sc}_1 = D_{\rm sc}\rho_{\rm sc}(0), \quad (48)$$

where $\rho_{\rm sc}(0) = 0.143t^{-1}$ is the bare DOS at $\tau = 0$, $\delta g_{\rm sc} = -0.346$, we have up to leading contribution

$$\Phi^{\rm sc}_1(\Delta_{\rm MIT}(\tau)) = (3t)^{-1}(D_{\rm sc}\rho_{\rm sc}(0)\ln(6/\tau) + \delta g_{\rm sc}), \quad (49)$$
$$\delta\mathcal{F}_{\rm sc}(\Delta_{\rm MIT}(\tau)) = -B_{\rm sc}\tau^2 t, \quad (50)$$

where $B_{\rm sc} = D_{\rm sc}\rho_{\rm sc}(0)/3 = 0.285$. We find $\delta\mathcal{E}_{\rm sc}(\tau) = -A_{\rm sc}\tau^2 t$, $A_{\rm sc} = 0.145$, so that $\delta\mathcal{F}_{\rm sc}(\tau) - \delta\mathcal{E}_{\rm sc}(\tau) < 0$. Thus, within the framework of HFA, we have a stable second-order transition curve for any $\tau \lesssim 0.5$, and the region of the AFM metal between the regions of the AFM insulator and the PM metal in the phase diagram is wide enough.

Numerical results on the $t' - U$ phase diagram for the sc lattice with $J = 0$ within both HFA and SBA approximations with account of non-collinear AFM (spiral) order are shown in Fig. 4 [2]. The transition is always of the second order and the AFM metal region is rather wide.

For the bcc lattice, despite the presence of Van Hove singularities, the situation is similar: at $J = 0$, a second-order transition is always realized. The stability boundary of the insulator AFM phase with respect to the PM phase in $\tau - \Delta$ variables, although non-linear (as for the square lattice), does not intersect with the transition line in the AFM metal [9].

The situation changes considerably for finite J, see Fig. 5. The correlation effects induced by an exchange interaction noticeably shift the position of first-order MIT for the square lattice (the size of the first-order τ-region can be made smaller (large) under the antiferromagnetic (ferromagnetic) exchange). For sc and bcc lattices, the nearest-neighbour ferromagnetic exchange $J \sim 0.5t$ can result in a first-order transition at $\tau > \tau_*(J)$, where $\tau_*(J)$ rapidly falls when J increases.

4. Conclusions

To conclude, the slave boson theory yields a physically reasonable description of the metal–insulator transition, the correlation effects playing an important role. The intersite Heisenberg interaction turns out to be important to describe the first-order transitions. Similar effects are expected from the intersite Coulomb interaction provided that we take into account charge density waves.

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6. References
[1] Katsnelson M I and Irkhin V Yu 1984 *J. Phys.* C **17** 4291
[2] Timirgazin M A, Igoshev P A, Arzhnikov A K, Irkhin V Yu 2016 *J. Low. Temp. Phys.* **185** 651
[3] Schüler M, van Loon E. G. C. P., Katsnelson M I, Wehling T O 2018 *Phys. Rev.* B **97** 165135
[4] Kotliar G and Ruckenstein A E 1986 *Phys. Rev. Lett.* **57** 1362
[5] Fresard R and Wölfle R 1992 *J. Phys.: Cond. Matt.* **4** 3625.
[6] Timirgazin M A, Igoshev P A, Arzhnikov A K, Irkhin V Yu 2016 *J. Phys.: Condens. Matter* **28** 505601
[7] Brinkman W F and Rice T M 1970 *Phys. Rev.* B **2** 4302
[8] Yu Z-Q and Yin L 2010 *Phys. Rev.* B **81** 195122
[9] Igoshev P A and Irkhin V Yu 2019 *J. Exp. Theor. Phys.* **128** 909